

On the application of Jucys-Murphy operators in the Hubbard model

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Abstract

The operator techniques based on the Jucys-Murphy operators were applied in the procedure of an immediate diagonalization of the one-dimensional Hubbard model. The Young orthogonal basis was given by the irreducible basis of the symmetric group acting on the set of nodes of the magnetic chain. The example of the attractive Hubbard model at the half-filled magnetic rings case was considered where the group $SU(2) \times SU(2)$ acts within the spin and pseudo-spin space. These techniques significantly reduced size of the eigenproblem of the Hubbard Hamiltonian.

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I. INTRODUCTION

Hubbard model [1], is the simplest generalization beyond the band theory description of solids, allowing us to understand many interesting phenomena of the solid state physics such as ferromagnetism, antiferromagnetism, the Mott transition, high-temperature superconductivity, Bose–Einstein condensate in cold optical lattice [2–5].

Despite being an approximation of the realistic electron interactions in a crystal, the results obtained with this model may explain insulating, magnetic, and even superconducting effects in solids, including 1D conductors.

In this paper one-dimensional Hubbard model is being considered [6]. Given the possibility of having exact solutions for this model [7–9] its importance is additionally magnified by the possibility of further generalization to higher dimensions. We consider the Young orthogonal basis, using the Jucys-Murphy operators [10–14] which represents the irreducible basis partially adapted to the total symmetry of the system. These operators generate a maximal Abelian subalgebra in the group algebra $\mathbb{C}[\Sigma_N]$ of the symmetric group, allowing us to interpret the orthogonal basis of standard Young tableaux as that of common eigenstates of a complete set of commuting operators [15, 16], in a frame of Dirac’s quantum-mechanical principles [17].

Considering that interacting particles are fermions, therefore, due to the exclusion principle, maximum of two particles are allowed to populate a single node. The electrons moving along the ring with N nodes labeled by the set $\tilde{N} = \{j = 1, 2, \dots, N\}$ have two possibilities of the one-node spin projection, namely $+\frac{1}{2}$ (denoted by $+$) and $-\frac{1}{2}$ (denoted by $-$), given by the set $\tilde{2} = \{i = +, -\}$. Since periodic boundary conditions are imposed one has to assume that $j + N = j$. We introduce two additional sets $\tilde{N}_i = \{j_i = 1, 2, \dots, N_i\}$, $i \in \{+, -\}$, with cardinality equal to the number of electrons with the spin projection in the set $\tilde{2}$, moving on the ring. The whole number of electrons is equal then $N_+ + N_- = N_e$, and is labeled by the set $\tilde{N}_e = \{j_e = 1, 2, \dots, N_e\}$. These electrons can hop to the nearest neighbours, provided the Pauli principle was not violated, and interact when two are on the same node, thus individual N_i numbers are conserved. Since we are dealing with the finite number of nodes of the lattice given by N , we assume the single band approximation.

II. THE HUBBARD HAMILTONIAN AND ITS SYMMETRIES

To get an insight into the dynamics of finite system of interacting electrons occupying the one-dimensional chain consisting of N atoms we use the Hubbard Hamiltonian of the following form

$$\hat{H} = t \sum_{i \in \tilde{2}} \sum_{j \in \tilde{N}} (\hat{a}_{ji}^\dagger \hat{a}_{j+1i} + \hat{a}_{j+1i}^\dagger \hat{a}_{ji}) + U \sum_{j \in \tilde{N}} \hat{n}_j + \hat{n}_j -, \quad (1)$$

where $\hat{n}_{ji} = \hat{a}_{ji}^\dagger \hat{a}_{ji}$, and \hat{a}_{ji}^\dagger , \hat{a}_{ji} are the canonical Fermi operators of creation and annihilation of an electron of spin i , on the site j .

The first component of the Hamiltonian (1) is responsible for the *wave-like* behaviour of the electrons, whereas the second component corresponds to the *particle-like* behaviour provided electron-electron interactions occur and are described by a characteristic interaction constant denoted by U [19]. In general U can be of any value, with $U < 0$ ($U \ll 0$ - the case presented in this article) and $U > 0$ ($U \gg 0$ [18, 20]) are responsible for attraction and repulsion, respectively. $U = 0$ stands for no effect for plain gas of fermions.

The *single-node* space h_j has the basis consisting of n vectors denoting all possible occupations of one node. For the fermions

$$\dim h_j = n = 4, \quad h_j = lc_{\mathbb{C}}\{\pm, \emptyset, +, -\}, \quad (2)$$

where \emptyset denotes the empty node, $+$ and $-$ stand for one-node spin projection equal to $\frac{1}{2}$ and $-\frac{1}{2}$, respectively, \pm denotes the double occupation of one node by two electrons with different spin projections, and $lc_{\mathbb{C}}A$ stands for the linear closure of a set A over the complex field \mathbb{C} .

The final Hilbert space \mathcal{H} of all quantum states of the system has the form

$$\mathcal{H} = \prod_{j=1}^N \otimes h_j, \quad \mathcal{H} = \sum_{N_e=0}^{2N} \oplus \mathcal{H}^{N_e}, \quad (3)$$

where \mathcal{H}^{N_e} denotes the space with fixed number of electrons N_e .

The initial, orthonormal basis of the Hilbert space \mathcal{H} consists of linearly independent vectors called *electron configurations* [21], defined by the following mapping

$$f : \tilde{N} \longrightarrow \tilde{4}, \quad \tilde{4} = \{\pm, \emptyset, +, -\}, \quad (4)$$

and constitute the N -sequences of the elements from the set $\tilde{4}$

$$|f\rangle = |f(1)f(2)\dots f(N)\rangle = |i_1 i_2 \dots i_N\rangle, \quad i_j \in \tilde{4}, \quad j \in \tilde{N}, \quad (5)$$

with

$$\tilde{4}^{\tilde{N}} = \{f : \tilde{N} \longrightarrow \tilde{4}\}, \quad (6)$$

$$\mathcal{H} = l_{\mathbb{C}} \tilde{4}^{\tilde{N}}. \quad (7)$$

Previously, work on problems related to the symmetries of the one-dimensional Hubbard model has appeared in the literature starting from Lieb and Wu [22], Yang [23] and continued in, inter alia, Refs. [19, 24, 25], with the book of Essler et al. being the eminent summary and supplement of their work [26].

Since the periodic boundary conditions are set, the Hamiltonian (1) has the obvious translational symmetry ($\hat{a}_{N+1i} = \hat{a}_{1i}$), therefore one-particle Hamiltonian of the form (1) is completely diagonalized by a Fourier transformation. Apart from the cyclic symmetry, system reveals, among others, two independent $SU(2)$ symmetries [26, 27], $SU(2) \times SU(2)$, in spin and pseudo-spin space [28]. This symmetry involves spin and charge degrees of freedom, thus one has two sets of generators, $\{\hat{S}_z, \hat{S}^+, \hat{S}^-\}$ and $\{\hat{J}_z, \hat{J}^+, \hat{J}^-\}$, for spin and charge respectively. These generators can be written in the following forms

$$\hat{S}_z = \frac{1}{2} \sum_{j \in \tilde{N}} (\hat{a}_{j+}^\dagger \hat{a}_{j+} - \hat{a}_{j-}^\dagger \hat{a}_{j-}), \quad \hat{S}_+ = \hat{S}_-^\dagger = \sum_{j \in \tilde{N}} \hat{a}_{j+}^\dagger \hat{a}_{j-}, \quad (8)$$

$$\hat{J}_z = \frac{1}{2} \sum_{j \in \tilde{N}} (\hat{a}_{j+}^\dagger \hat{a}_{j+} + \hat{a}_{j-}^\dagger \hat{a}_{j-} - 1), \quad \hat{J}_+ = \sum_{j \in \tilde{N}} (-1)^j \hat{a}_{j+}^\dagger \hat{a}_{j-}^\dagger, \quad \hat{J}_- = \sum_{j \in \tilde{N}} (-1)^j \hat{a}_{j+} \hat{a}_{j-} \quad (9)$$

and the transfer between these two sets is known as the Shiba transformation from the mapping rotations in spin space into rotations in pseudo-spin space, achieved by changing the sign of U [22, 26].

III. JUCYS-MURPHY OPERATORS

The operators \hat{M}_j , defined within the symmetric group algebra $\mathbb{C}[\Sigma_N]$ as the sum of all transpositions (j, j') of the node $j \in \tilde{N}$ with preceding nodes $j' < j$, were introduced by Jucys [10, 11] and independently by Murphy [12]. These correspond to $N - 1$ hermitian and

mutually commuting operators of the form

$$\hat{M}_j = \sum_{1 \leq j' < j} (j, j'), \quad j = 2, 3, \dots, N, \quad (10)$$

which generate a maximal Abelian subalgebra in $\mathbb{C}[\Sigma_N]$. The standard Young tableaux $|\lambda_N y \rangle$ [29] of the shape $\lambda_N \vdash N$, i.e. the tableaux of this shape in the alphabet \tilde{N} of nodes, with strictly increasing entries in rows and columns, constitutes the common eigenvector $|\lambda_N y \rangle$ of the set of \hat{M}_j operators, that is

$$\hat{M}_j |\lambda_N y \rangle = m_j(y) |\lambda_N y \rangle, \quad (11)$$

with eigenvalues

$$m_j(y) = c_j(y) - r_j(y), \quad (12)$$

where the pair of positive integers $(c_j(y), r_j(y))$ gives the positions (the column and the row) of the number j in tableaux $|\lambda_N y \rangle$.

This leads to each basis function of the irreducible representation Δ^{λ_N} of the symmetric group Σ_N , labeled by the Young tableaux $|\lambda_N y \rangle$, being completely determined by the sequence $(m_1 = 1, m_2, \dots, m_N)$ of eigenvalues (12). The realization of each such irreducible vector within the group algebra $\mathbb{C}[\Sigma_N]$ is given via the projection operator $e_{yy}^{\lambda_N}$ of the well known Young orthogonal basis [10–12], where the importance of the Jucys-Murphy operators is underlined.

IV. THE IRREDUCIBLE BASIS

Since the system of the half-filling magnetic ring reveals two independent $SU(2)$ symmetries [26, 27] $SU(2) \times SU(2)$ - the spin and the charge degrees of freedom (called *particles*) are possible in the spin and the pseudo-spin space, respectively.

Assuming there is only one particle on the ring we allow the symmetric group Σ_N act on the number of nodes N . The set of all allowed positions of the particle at N nodes forms the orbit O_μ of the symmetric group Σ_N , labeled by the weight [22] $\mu = (\mu_1, \mu_2)$, where $\mu_1 = N - 1$ and, since there is only one particle in the system, $\mu_2 = 1$. Such an orbit is invariant under the action of the symmetric group Σ_N and forms the carrier space of the transitive representation $R^{\Sigma_N: \Sigma^\mu}$, with the stabilizer Σ^μ being the Young subgroup $\Sigma^\mu = \Sigma_{\mu_1} \times \Sigma_{\mu_2}$, where \times denotes the Cartesian product.

One can obtain states with definite permutational symmetry of the N_p particles of one kind contained either within the spin space or within the pseudo-spin space by taking the irreducible basis of the appropriate irreducible representations Δ^{λ_N} of the symmetric group Σ_N , where $\lambda_N \vdash N$, in the tensor products of N_p transitive representations $R^{\Sigma_N: \Sigma^{(N-1,1)}}$ along with the appropriate decomposition

$$R^{\Sigma_N: \Sigma^\mu} \cong \sum_{\lambda_N \supseteq \mu} K_{\lambda_N \mu} \Delta^{\lambda_N}. \quad (13)$$

Here $K_{\lambda_N \mu}$ corresponds to the Kostka numbers [30], and the sum runs over all partitions λ_N greater than or equal to μ in the dominance order [31].

In order to obtain Young orthogonal basis [10–12] of the tensor product of the appropriate transitive representations

$$(R^{\Sigma_N: \Sigma^{(N-1,1)}})^{\otimes N_p}, \quad (14)$$

with the decomposition into irreducible representations Δ^{λ_N} given by equation (13), we are going to use Jucys-Murphy operators and create the projection operators

$$e_{yy}^{\lambda_N} = |\lambda_N w y\rangle \langle \lambda_N w y| \quad (15)$$

in the space of the tensor product $(h_j)^{\lambda_{N_p}}$. Here w is an appropriate repetition label and $y \in SYT(\lambda_N)$, with $SYT(\lambda_N)$ being the set of all standard Young tableaux of the shape λ_N .

Thus we have

$$e_{yy}^{\lambda_N} = \prod_{j=2}^N \prod_{\{y_{j-1} | y_{j-1}^+ \neq y_j\}} \frac{\hat{M}_j - m_j(y_{j-1}^+) \hat{I}}{m_j(y) - m_j(y_{j-1}^+)}, \quad (16)$$

with $y \in SYT(\lambda_N)$ and y_j corresponding to the tableaux obtained from y by extracting the set $\{j+1, j+2, \dots, N\}$ of numbers. y_{j-1}^+ can be created from y_{j-1} after adding to its entries the number j , and \hat{I} stands for the appropriate unity operator.

V. THE EXAMPLE

As discussed in the previous section the system of the half-filling magnetic ring reveals, among others, two independent $SU(2)$ symmetries, allowing us to use the above technique for the pseudo-spin space [28].

The set of electron configurations for the attractive Hubbard model corresponding to $U \ll 0$ [32], does not contain the elements with two atoms singly occupied by opposite spin projection (unpaired spins) and thereby provides the charge degrees of freedom only.

Consider the irreducible basis for the half-filling case of $N = 4$, $N_- = 1$, and $U \ll 0$ in the form

$$R^{\Sigma_4:\Sigma(3,1)} \otimes R^{\Sigma_4:\Sigma(3,1)} = R^{\Sigma_4:\Sigma(3,1)} \oplus R^{\Sigma_4:\Sigma(2,1^2)} \quad (17)$$

of the transitive representations with appropriate decomposition into irreducible representations Δ^λ given by

$$R^{\Sigma_4:\Sigma(3,1)} = \Delta^{\{4\}} \oplus \Delta^{\{3,1\}}, \quad (18)$$

and

$$(\Delta^{\{4\}} \oplus \Delta^{\{3,1\}}) \otimes (\Delta^{\{4\}} \oplus \Delta^{\{3,1\}}) = 2\Delta^{\{4\}} \oplus 3\Delta^{\{3,1\}} \oplus \Delta^{\{2^2\}} \oplus \Delta^{\{2,1^2\}}. \quad (19)$$

States related to the first component on the right-hand side of the tensor product in decomposition (17) describe the situation corresponding to the occupancy of a single node by two particles and are therefore to be rejected due to impossibility of combining \pm and \emptyset together into the single one-node state.

The transitive representation $R^{\Sigma_4:\Sigma(2,1^2)}$ contains the symmetric

$$(R^{\Sigma_4:\Sigma(2,1^2)})_{st} = \Delta^{\{4\}} \oplus \Delta^{\{3,1\}} \oplus \Delta^{\{2^2\}}, \quad (20)$$

and the antisymmetric

$$(R^{\Sigma_4:\Sigma(2,1^2)})_a = \Delta^{\{3,1\}} \oplus \Delta^{\{2,1^2\}}, \quad (21)$$

part of the tensor product (17). The decompositions of selected elements of the irreducible basis of the symmetric group Σ_4 onto the electron configurations are presented in Table I.

According to (20) and (21) application of the irreducible basis to the 12-dimensional Hubbard Hamiltonian for the case of $N = 4 = N_e$, $N_- = 1$, leads to the quasidiagonal form with three three-dimensional, and three one-dimensional blocks on the diagonal.

VI. CONCLUSIONS

We have demonstrated the applications of the Young irreducible basis in the diagonalization procedure of the one-dimensional Hubbard model, using the set of Jucys-Murphy operators.

$ f\rangle$	$\begin{array}{ c c }\hline 1 & 3 \\ \hline 2 & 4 \\ \hline\end{array}$		$\begin{array}{ c c }\hline 1 & 2 \\ \hline 3 & 4 \\ \hline\end{array}$		$\begin{array}{ c c }\hline 1 & 3 \\ \hline 2 & 4 \\ \hline\end{array}$		$\begin{array}{ c c }\hline 1 & 4 \\ \hline 2 & 3 \\ \hline\end{array}$	
$\pm\emptyset++$	0	$\frac{1}{\sqrt{6}}$	0	$\frac{1}{2\sqrt{3}}$	$\frac{-1}{\sqrt{6}}$			
$\pm+\emptyset+$	$\frac{1}{2\sqrt{2}}$	$\frac{-1}{2\sqrt{6}}$	$\frac{1}{4}$	$\frac{1}{4\sqrt{3}}$	$\frac{1}{\sqrt{6}}$			
$\pm++\emptyset$	$\frac{-1}{2\sqrt{2}}$	$\frac{-1}{2\sqrt{6}}$	$\frac{-1}{4}$	$\frac{-\sqrt{3}}{4}$	0			
$\emptyset\pm++$	0	$\frac{1}{\sqrt{6}}$	0	$\frac{-1}{2\sqrt{3}}$	$\frac{1}{\sqrt{6}}$			
$+\pm\emptyset+$	$\frac{-1}{2\sqrt{2}}$	$\frac{-1}{2\sqrt{6}}$	$\frac{1}{4}$	$\frac{-1}{4\sqrt{3}}$	$\frac{-1}{\sqrt{6}}$			
$+\pm+\emptyset$	$\frac{1}{2\sqrt{2}}$	$\frac{-1}{2\sqrt{6}}$	$\frac{-1}{4}$	$\frac{\sqrt{3}}{4}$	0			
$\emptyset+\pm+$	$\frac{1}{2\sqrt{2}}$	$\frac{-1}{2\sqrt{6}}$	$\frac{-1}{4}$	$\frac{-1}{4\sqrt{3}}$	$\frac{-1}{\sqrt{6}}$			
$+\emptyset\pm+$	$\frac{-1}{2\sqrt{2}}$	$\frac{-1}{2\sqrt{6}}$	$\frac{-1}{4}$	$\frac{1}{4\sqrt{3}}$	$\frac{1}{\sqrt{6}}$			
$++\pm\emptyset$	0	$\frac{1}{\sqrt{6}}$	$\frac{1}{2}$	0	0			
$\emptyset++\pm$	$\frac{-1}{2\sqrt{2}}$	$\frac{-1}{2\sqrt{6}}$	$\frac{1}{4}$	$\frac{\sqrt{3}}{4}$	0			
$+\emptyset+\pm$	$\frac{1}{2\sqrt{2}}$	$\frac{-1}{2\sqrt{6}}$	$\frac{1}{4}$	$\frac{-\sqrt{3}}{4}$	0			
$++\emptyset\pm$	0	$\frac{1}{\sqrt{6}}$	$\frac{-1}{2}$	0	0			

TABLE I. The irreducible basis (columns 2 - 6) of the representations $\Delta^{\{2^2\}}$ and $\Delta^{\{2,1^2\}}$ of the symmetric group Σ_4 taken as the linear combinations of the electron configurations of the first column.

We have shown the way of finding the basis with definite permutational symmetry based on the properties of the maximal Abelian subalgebra in the group algebra $\mathbb{C}[\Sigma_N]$ of the symmetric group Σ_N .

We explored the example of an attractive Hubbard model ($U \ll 0$) and the half-filling magnetic rings with N nodes occupied by $N_e = N$ electrons, including $N - 1$ electrons with the same spin projection.

This approach leads to a significant reduction in the size of the Hubbard Hamiltonian and the result obtained for the projection operators of the Young orthogonal bases can easily be implemented into numerical simulations due to the use of simple transpositions being the generators of the symmetric group.

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